Development of Li-metal battery cell chemistries at NASA Glenn Research Center

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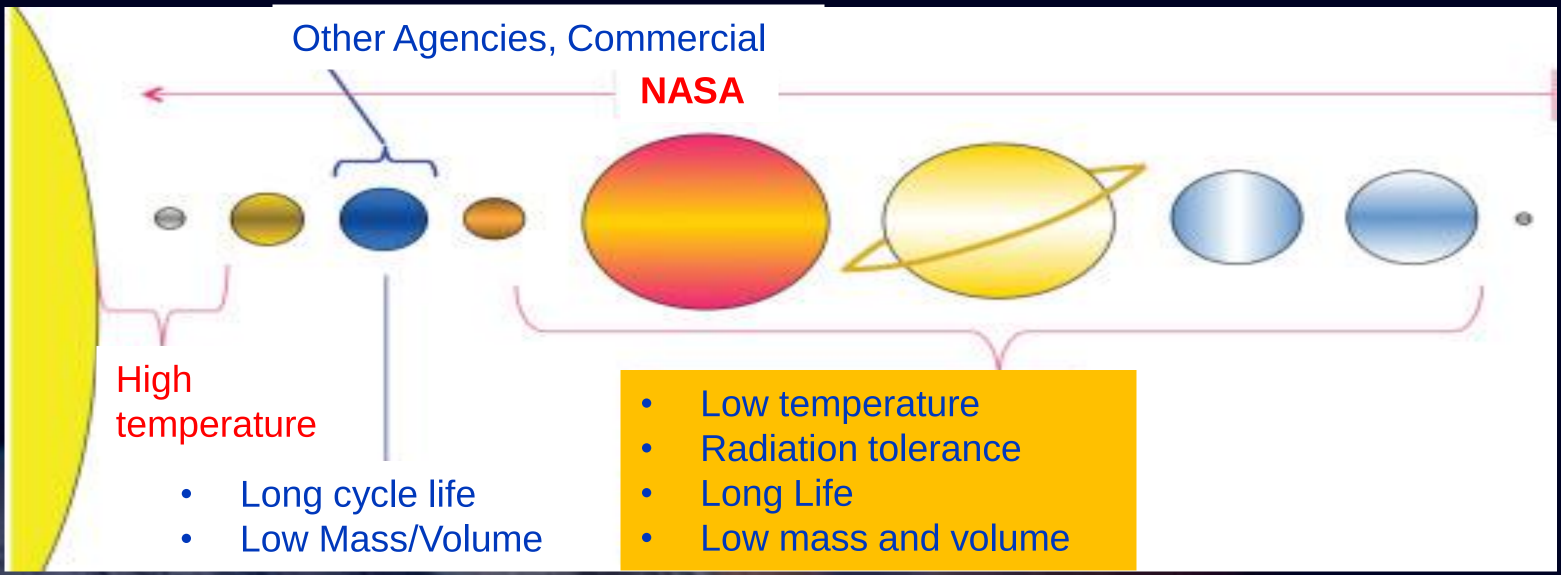
NASA Goals in Batteries and Energy Storage



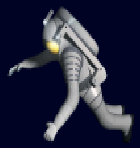
NASA's energy storage needs span a greater range of environments and cycle requirements than other organization's applications.

Energy storage technologies are core to every space mission, and their mass is often referred as a barrier to achieving mass efficient systems

Several key NASA applications require very high specific energy (>500 Wh/kg) with enhanced safety, while commercial HEV-driven market requires low cost, long cycle life, with specific energy ~250 Wh/kg.

High Specific Energy Batteries

Power Systems NASA Roadmap



Advanced EVA Systems

Habitat Lander (crewed descent)

Surface Systems

Robotic Assistants & Devices

Teleoperated Robots

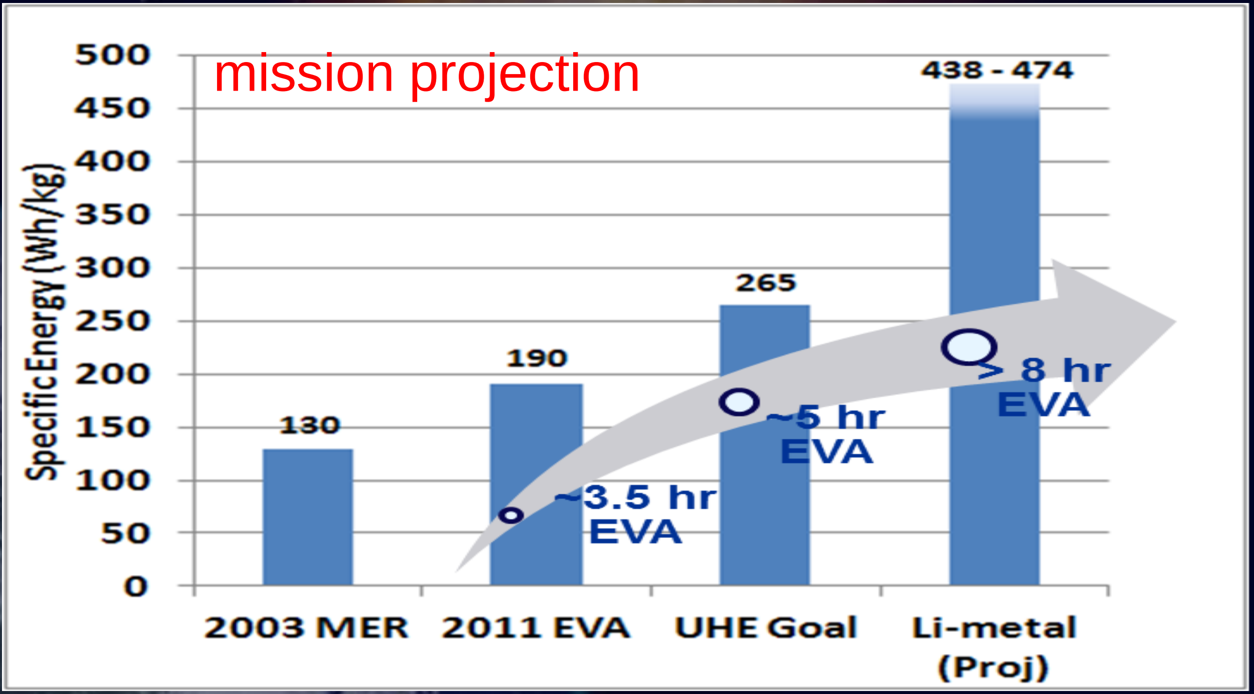
- Applicable to these Capabilities/Elements; Destinations/Con-Ops
  - Driving: ExtraVehicle Activity (EVA), In-Space Robotics; Cis-lunar missions
  - Beneficiary: Lander, Surface Elements for Lunar and Mars, hybrid eletric aviation, SmallSats

- EVA battery Performance characteristics
  - Battery-level specific energy > 325 Wh/kg and energy density > 540 Wh/liter
  - 8 hour operation per mission over an operating temperature of 10 to 30 degrees C.
  - Nominally 100 cycles and 5 year calendar life

- Description
  - Batteries with very high specific energy and energy density are required to enable EVA missions. Batteries are expected to provide sufficient power for life support and communications systems, and tools including video and lighting. Advanced batteries are enhancing for several other missions.

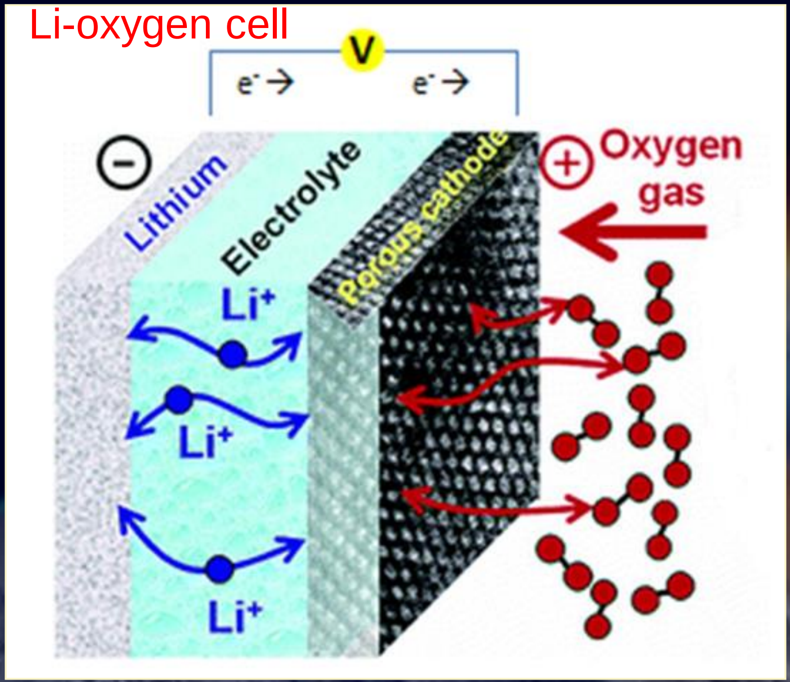
Status Quo and Where We Need to Go

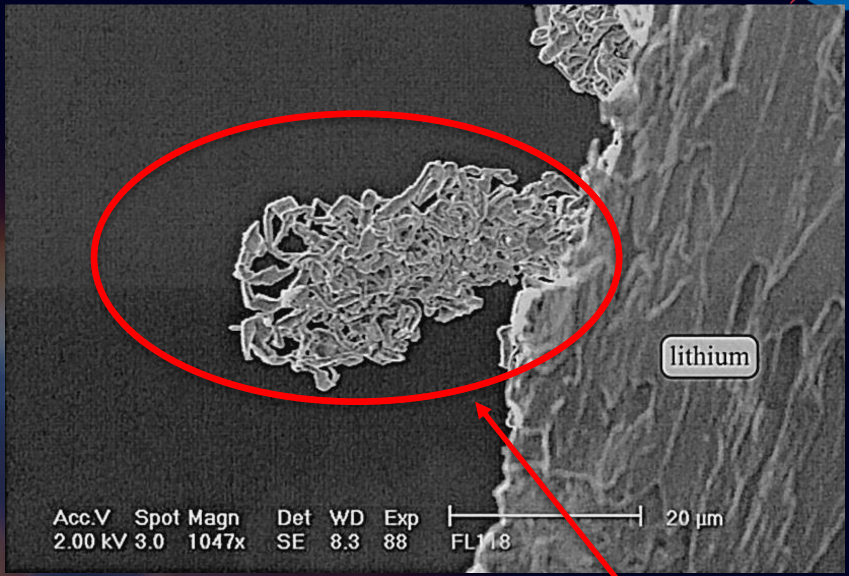
- Li-ion cell technology is relatively new to aerospace (within the past 10 years), and although it offers 2-3 X times improvement in specific energy over its Ni-based counterparts, space applications still demand much higher specific energy
- SOA Li-ion cells that were used for the EVA battery demonstration in 2012 achieved 190 Wh/kg;
- Li-ion technology used in MER Rovers achieved 130 Wh/kg with "low temperature" electrolyte;
- Advanced Li-ion technology developments have a goal value of ~ 265 Wh/kg at the cell level at 10 ^{0}C.



Need investment in development of disruptive, ultra high energy density "Beyond Li ion" technologies delivering cells with 3X-5X increase in specific energy, maintaining safety and cycle life.

"Beyond Li-ion" Battery Chemistries





Battery failure due to dendrites

F. Orsini et al., J. Power Sources 76, 19-29 (1998)

- **Advantage:** Lithium metal anode has ***10X*** increase in specific energy relative to graphite (in theory)
- Lithium metal anodes combined with **advanced cathodes** could achieve up to 1000 Wh/kg in cell specific energy, and realistically short-term ~ 400 Wh/kg.
- **Disadvantage:** *safety* and *cycling* possibly worse than LIB
- Solution to "Li metal problem" is the *Holy Grail* of advanced battery technology
- Efficient cycling of Li-metal is crucial for realizing Li/S, Li/O_2 and other Li-metal chemistries

Rechargeable **batteries with Li metal anodes are not currently practical due to** ***cell components' integration, electrode-electrolyte kinetics***, ***electrolyte decomposition*** ***challenges***

Focus: Li-sulfur Battery Development

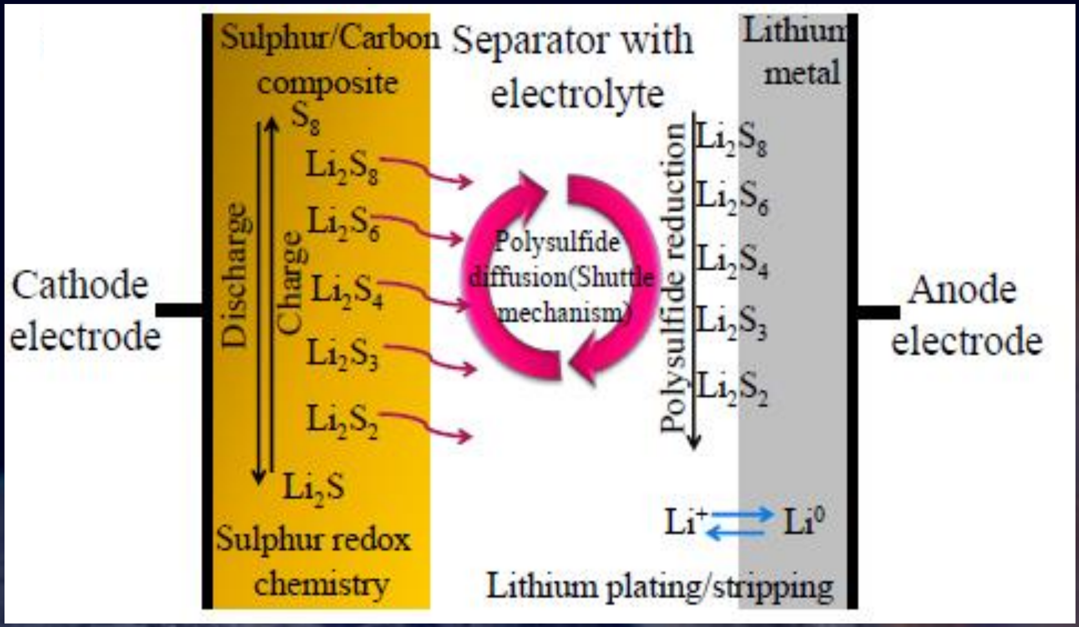


Image- provided by Storagenergy Technologies Inc

- Poor cycle life due to fast capacity degradation: formation of **soluble polysulfide**, L_2S_n
- Poor electrode rechargeability and limited rate capability: the **insulating nature** of sulfur
- Low sulfur utilization: **insoluble** Li_2S and Li_2S_2
- A poorly understood **Li/electrolyte interface**: dendrite formation

- Need to develop better understanding of Lithium/Sulfur system kinetics and interactions
- Cell component integration, new cathodes, and specialized electrolytes are required to solve cell performance problems such as “polysulfide shuttle” and safety.
- Computational modeling approaches to assist and guide fundamental development process
- The combination of new materials synthesis, computational modeling, performance analysis and testing are required
- NASA investments in SBIRs, NASA Research Announcements (NRA)
- Partnerships with DOE, ARPA-E

NASA Investment Strategy - Advancing Batteries and Cell Technologies

- NASA invested in the development of high energy Li-ion and “Beyond Li-ion”:
  - Multi-phase SBIRs, STTRs, EPSCORs funded by
    - **Human Exploration and Operations Mission Directorate (HEOMD)**
    - **Space Technology Mission Directorate (STMD)**
    - **Science Mission Directorate (SMD)**
  - NRAs such as Advanced Energy Storage Systems (AESS), funded by
    - **Space Technology Mission Directorate (STMD)**
  - Internal NASA cell research and battery engineering funded by
    - **Space Technology Mission Directorate (STMD)**
    - **Aeronautics Research Mission Directorate (ARMD)**
  - Collaborations with Government, Academic, and Industry partners.
- NASA team developed internal capabilities in Li-metal component development and integration, computational modeling, and cell design and validation.
- These multi-phase activities will result in the development of advanced Li-ion and “Beyond Li-ion” battery cell chemistries.
- NASA team leads the technology infusion effort, supporting missions such as EVA and Mars surface exploration

NASA Battery SBIR, STTR, EPSCOR programs

2014 Phase I SBIR – Funding of up to $125K for 6 months, 17 Awards

2014/2015 Phase II SBIR – Funding of up to $750K for 24 months, 3 Awards

2014/15 EPSCOR – Funding of up to $750K for 36 months, 3 Awards

- NASA SBIR topics are aligned with Mission Directorates
  - Solicitations focus on technology gaps specific to the particular mission directorate

- Subtopics in FY14 solicitation with focus on electrochemical technologies led by NASA Glenn Research Center:
  - Human Exploration and Operations Mission Directorate
    - Advanced Next Generation Batteries
  - Space Technology Mission Directorate
    - Advanced Space Battery Technology
  - Science Mission Directorate
    - Power Electronics and Management, and Energy Storage

SBIRs offer opportunities to develop, evaluate and leverage technologies for infusion into future NASA missions

Advanced Energy Storage Systems (AESS) Program

Technology Development Phase	TRL at end of Phase (Cat. One)	TRL at end of Phase (Cat. Two)	Anticipated Number of Awards*	Value of Each Award	Period of Performance (POP)
Phase I	4	3	4	Up to $250K per	Up to 8 Months
Phase II	5	4	2	Up to $1M per	Up to 12 Months
Phase III	6	5	1	Up to $2M	Up to 15 months

- Category 1, “High Specific Energy System Level Concepts” - focus on maturation of system level battery technologies such as packaging and cell integration.
- Category 2, “Very High Specific Energy Devices” - focus on energy storage technologies that have the potential to go beyond present capabilities characterized by Li^+ chemistry, while maintaining the required duty cycle and safety of any system operating in space.
- Work under AESS is synergistic with ongoing efforts within other Government Agencies.
- Full cell deliverables after Phase I in May 2015.
- “Scaled-up” full cells, battery design and brassboard deliverables after Phases II & III in 2016/2017.

AESS Program offers opportunities to develop, evaluate, mature, and leverage technologies for infusion into future NASA missions

NASA Battery Program Portfolio in Advanced Batteries, Cells, and Components

- Advanced Li-ion
- Li/Sulfur with liquid electrolyte
- Li/Sulfur with solid electrolyte
- Advanced components
- Battery systems

- Amprius*
- PH Matter
- PSI
- IUPUI*
- Storagenergy
- Bettergy
- NOHMs
- JPL/CalTech*
- Yardney
- University of Maryland*
- Solid Power
- Cornerstone Research
- TH Chem
- Poly-K
- NEI
- Materials Modifications
- Xerion
- American Energy
- Giner
- Illinois Rocstar
- Applied Materials Systems
- Iowa State University#
- University of South Dakota#
- Missouri University of S&T#

* - AESS Program Awards

- EPSCOR Program Awards

This Program portfolio is leveraged through NASA internal research and engineering efforts for infusion of cutting edge battery technologies for several NASA missions such as *EVA spacesuit, exploration rovers, landers, electric aviation, and SmallSats*.

NASA Internal Research: Novel Electrolytes in Lithium Metal Systems

Possibilities for new electrolytes

- ❑ **Ionic liquids**
- ❑ **Solid electrolytes – ceramic and polymer**

Model Study (2012-2015) funded by ARMD: New Ionic Liquid Electrolyte design

- **Electrolyte selection is critical for Li metal battery performance**
- **Model system**: Ionic liquids
- Many highly stable (rechargeable) and non-flammable (safe)
- ***Stability*** **is critical for battery rechargeability & cycle life**
- **Some ILs are stable against Li metal decomposition; however, others are not. Why?**
- Many *other* properties required for viable electrolyte
- Vast number of ILs possible ~10^{18}
- **Chemical design/synthesis of new ILs with tailored properties possible**

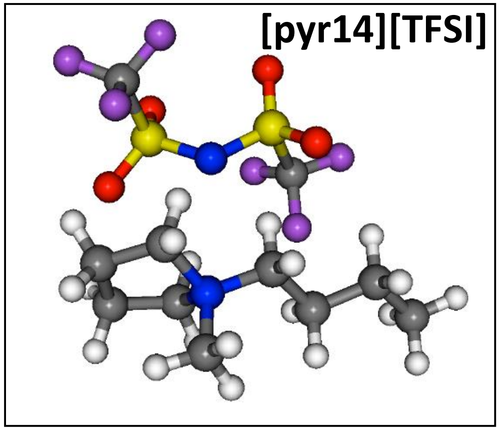
Cross-Center, Multi-Disciplinary Team

NASA Ames Computational Materials Group: modern computational material science and computational chemistry

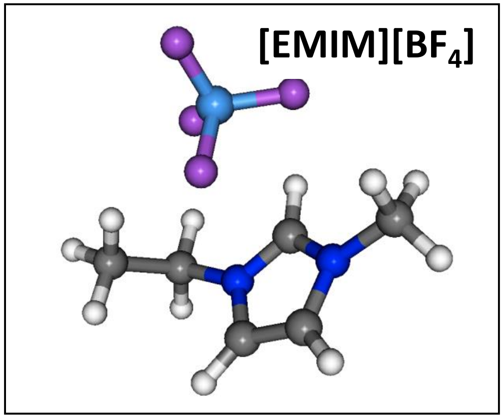
NASA Glenn PV & Electrochemistry Branch: wide-ranging experience in battery development and experimental characterization

Ultimate goal: determine *electrolyte design rules* for high energy, rechargeable, safe batteries

Good Stability



Poor Stability



Bhattacharyya et al., Nat. Mat. 9, (2010), p 504

Technical Goals for the Model Study Program

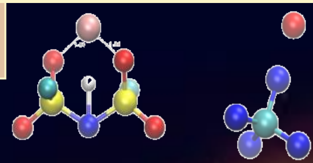
- **Technical Questions:**
  - Is IL ionic conductivity too low for batteries?
  - What is the detailed interaction between IL electrolyte and Li metal anode?
  - What is the cell performance with ILs and Li metal electrodes?
  - What is the detailed interaction between IL electrolyte and cathode materials?
  - What is the optimal electrolyte?
  - How to optimize the components integration into a functioning full cell?
  - Understanding of all these issues is incomplete for SOA LIB after >20 years

- **Innovation:** *develop <u>unique</u> set of computational tools tightly coupled with experiments to accelerate fundamental understanding, screening and design of novel electrolytes for complex, advanced batteries*

- **Benefit/Impact:** accelerated development of high energy, safe, rechargeable batteries

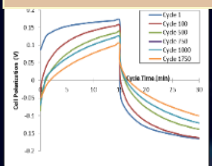
Model Study Program Summary

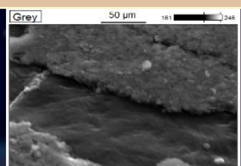
I. Ionic Liquids Electrolytes



- Molecular simulations of IL ionic conductivity
- Determined detailed structure and properties of three bulk ILs electrolytes
- Electrolyte Ionic Conductivity, Diffusion & Viscosity validation

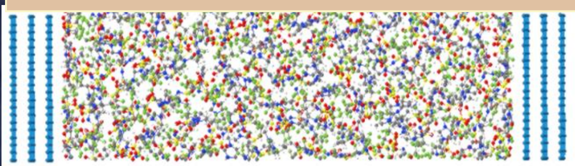
II. Experimental Cell Characterization





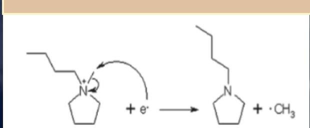
- Built and fully characterize <u>half</u> cells with IL electrolytes (cycling, impedance, voltammetry, SEM/EDAX)
- Surface layer identification for various electrolytes
- Identified class of IL electrolytes with stable cycling

III. Ionic Liquid-Electrode interface



- Implemented high accuracy polarizable force fields for Electrode-IL electrolyte interface simulations and
- Electric double layer structure/properties under applied voltage
- Correlated molecular structure with measured differential capacitance quantitatively
- Identified surface decomposition reactions

IV. Interfacial chemistry

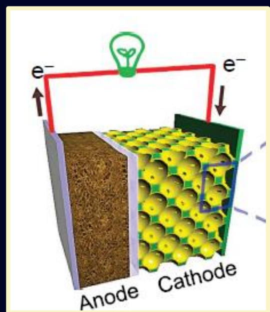


- IL electrolyte-surface decomposition conditions identified
- Correlated morphology of surface layer with cycling performance
- Analyzed electron transfer of molecule as a function of voltage
- Identified chemical pathways and mechanisms

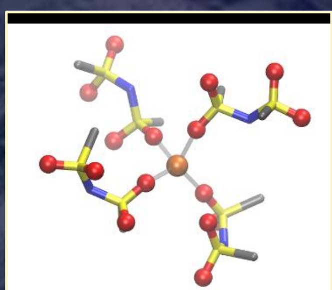
V. Li-Air cell demonstration

- Build Li-oxygen coin cell with “preferred” IL electrolyte
- 160 shallow cycles achieved
- 126 days of exposure to dry-room air

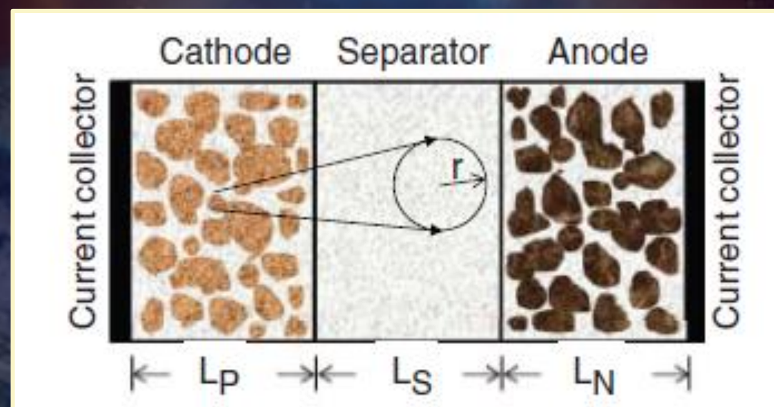
NASA GRC / ARC Development of Multi-Scale Battery Modeling Toolkit



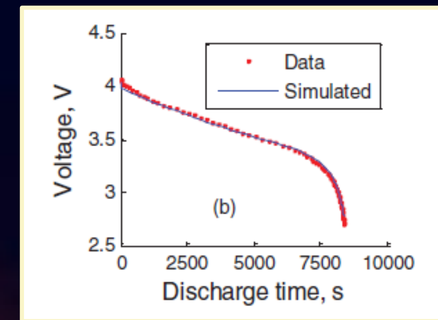
Microstructure Design



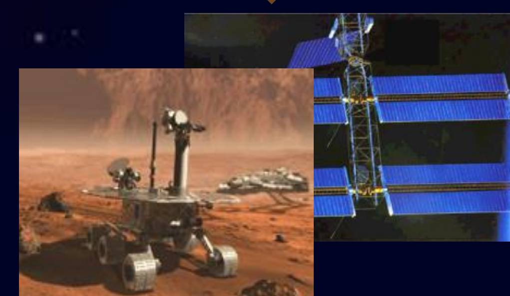
Chemical Design



Multi-Physics Cell Design



Cell Simulation

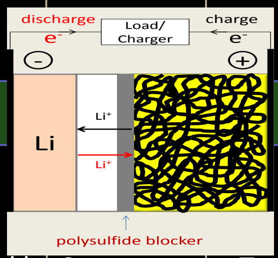


Space Technology Applications

Batteries require multiple levels of design: _chemical design_ of electrolytes and electrode materials, _microstructural design_ of electrodes, and _cell level_ component selection, sizing and performance simulations. Optimize designs for space missions requirements.

High Energy Battery Technology Maturation Roadmap

Materials Development (Cathode, Anode and Electrolyte)



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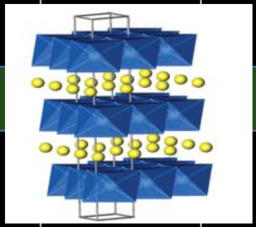


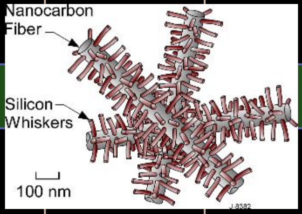
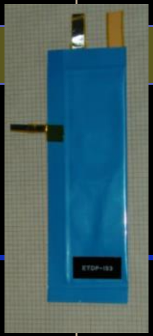
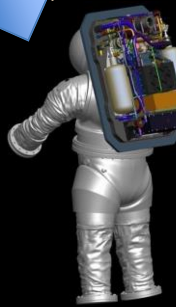


Image- provided by PSI

Cell Development and Scale-up



Battery Pack Demonstration



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Thanks for your attention!